A microscopic approach to phase transitions in quantum systems

Pietro Gianinetti[1,2] and Alberto Parola[1,3] *

[1] *Istituto Nazionale per la Fisica della Materia*
[2] *Dipartimento di Fisica, Universitá di Milano, Via Celoria 16, Milano, Italy*
[3] *Dipartimento di Scienze Fisiche, Universitá dell'Insubria, Via Lucini 3 Como, Italy*

We present a new theoretical approach for the study of the phase diagram of interacting quantum particles: bosons, fermions or spins. In the neighborhood of a phase transition, the expected renormalization group structure is recovered both near the upper and lower critical dimension. Information on the microscopic hamiltonian is also retained and no mapping to effective field theories is needed. A simple approximation to our formally exact equations is studied for the spin-S Heisenberg model in three dimensions where explicit results for critical exponents, critical temperature and coexistence curve are obtained.

Several physical systems, ranging from magnets to superfluids and superconductors, display rich phase diagrams in a temperature regime where quantum effects cannot be neglected. Different scenarios, characterized by competing order parameters and zero temperature phase transitions have been recently advocated also in the framework of high temperature superconductivity where antiferromagnetic order, Cooper pairing and, possibly, phase separation are at play in the same region of the phase diagram [1]. A satisfactory understanding of phase transitions in quantum models has been attained years ago through the seminal work by Hertz [2] who showed that, at low energy and long wavelengths, quantum models may be described by a suitable classical action. However, a quantitative theory of the thermodynamic behavior is still lacking and we mostly rely on mean field approaches or weak coupling renormalization group (RG) calculations [3], applied to quantum systems via the mapping to the appropriate effective field theory. In particular, the interplay between thermal and quantum fluctuations is expected to give rise to crossover phenomena whose extent strongly depends on the microscopic features of the system. Even for the most extensively studied models, like the Heisenberg antiferromagnet, our knowledge of the phase diagram is in fact limited, and the first precise finite temperature simulation attempting to fill this gap has become available only recently [4]. By contrast, in classical models, numerical simulations are quite efficient even in the neighborhood of critical points [5] and, from the analytical side, microscopic approaches especially devised for the quantitative description of the phase diagram of classical fluids and magnets are available. For instance, the hierarchical reference theory of fluids (HRT) [6] has proven quite accurate in locating the phase transition lines both in lattice and in continuous models.

In this Letter we sketch the derivation of the quantum hierarchical reference theory of fluids (QHRT) which we then apply to the Heisenberg antiferromagnet. We will demonstrate that the known renormalization group equations near four and near two dimensions are naturally recovered within our approach, which therefore unifies two complimentary techniques. On approaching the critical point, the spin velocity vanishes according to the expected dynamical critical exponent for an antiferromagnet. Finally, the phase diagram of this model in three dimensions is computed by numerical integration of a simple approximation to the the QHRT equations, providing a concrete application of our general approach.

The starting point is a microscopic, many body hamiltonian H written as the sum of a reference part H_0 and an interaction term V. The interaction is assumed to be bilinear in some operator $\rho(r)$, which is assumed either linear in bosonic operators or quadratic in fermionic ones:

$$V = \frac{1}{2} \int dx dy \rho(x) w(x-y) \rho(y) \tag{1}$$

with a non singular (i.e. Fourier transformable) two body potential w. The properties of the reference system under the action of an external field h coupled to the order parameter $\rho(r)$ are supposed known. No specific assumption on the reference system is made: in particular we do not need that H_0 corresponds to a non interacting system, where Wick theorem applies (such a feature is crucial in setting up the QHRT equations). These requirements are indeed rather general and include several models of current interest in many body physics: quantum magnets (where $\rho(r)$ represents the local spin variable), fermionic systems, like the Hubbard model, or even the Holstein model for the electron-phonon problem.

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*Fax: +39-02-2392482, e-mail: parola@mi.infm.it

The first task is to build up a formal perturbative expansion of the partition function of the model: $Z = \mathrm{Tr}\exp(-\beta H)$. Following a standard procedure [7], Z/Z_0 can be written as the average over the reference distribution function of an imaginary time evolution operator $U(\beta)$. When this operator is written as a power series of the interaction $w(r)$, we formally recover a perturbative expansion identical to that of a classical partition function for a $(d+1)$ dimensional model. The additional "temporal" dimension is limited to the interval $(0,\beta)$ and $w(r)\delta(t)/\beta$ plays the role of classical two body interaction $w_c(r,t)$. The reference system of the associated classical model is implicitly defined by requiring that its correlation functions coincide with those of the quantum reference hamiltonian H_0. *Approximate* mappings between a quantum model and an effective classical system have been proposed and studied in the literature [8] in order to clarify the role of thermal and quantum fluctuations. The novelty of our approach is that *i*) it is *exact* and *ii*) it applies to all temperature regimes, including the $T \to 0$ limit. Having reduced the quantum problem to a classical one, we can directly apply the techniques developed in that framework. In particular, the already mentioned HRT is an implementation of the momentum space renormalization method which preserves information on the details of the microscopic hamiltonian. In HRT, different Fourier components of the two body interaction are included gradually, starting from the shortest wavelength: physically this corresponds to a smooth turning on of fluctuations over larger and larger lengthscales. This procedure can be carried out exactly by defining a sequence of auxiliary systems interacting via a potential whose Fourier components coincide with $w(k)$ for $k > Q$ and vanish elsewhere. As a result, we obtain a set of coupled differential equations expressing the change in the free energy and in the correlation functions of the model when a given Fourier component Q of the potential is included. The initial condition represents the system in which fluctuations are frozen, and in fact coincides with the known mean field result. As the *cut-off* wavevector $Q \to 0$, the fully interacting system is recovered. Mean field *approximation* therefore corresponds to neglecting the change in the properties of the model as described by our differential equations. Details can be found in Ref. [6].

As an example, we study the the spin-S antiferromagnetic Heisenberg model on a hypercubic lattice in d dimension:

$$H = H_0 + V = h\sum_{\mathbf{R}} e^{i\mathbf{g}\cdot\mathbf{R}} S_{\mathbf{R}}^z + J\sum_{<\mathbf{R},\mathbf{R}'>} \mathbf{S}_{\mathbf{R}}\cdot\mathbf{S}_{\mathbf{R}'} \tag{2}$$

where the sum is restricted to nearest neighbors and $\mathbf{g}$ is the antiferromagnetic wavevector of components $g_i = \pi$. In applying the HRT approach to a quantum model, we decided to impose the cut-off Q only to the spatial Fourier components of $w_c(r,t)$. Different physical models might require other choices of the cut-off, whose only role is to continuously connect the reference system to the fully interacting one, which is recovered in the $Q \to 0$ limit. The exact evolution equation for the Helmholtz free energy density a of the system describes how a is modified due to a change in the cut-off Q:

$$\frac{d\,a^Q}{dQ} = \frac{1}{2\beta}\int_{\mathbf{p}\in\Sigma_Q}\sum_{\omega}\left\{2\ln\left[(1-F_{xx}^Q(\mathbf{p},\omega)w(\mathbf{p}))(1+F_{xx}^Q(\mathbf{p}',\omega)w(\mathbf{p})) - F_{xy}^Q(\mathbf{p},\omega)F_{xy}^Q(\mathbf{p}',\omega)w(\mathbf{p})^2\right]\right.$$
$$\left. + \ln\left[(1-F_{zz}^Q(\mathbf{p},\omega)w(\mathbf{p}))(1+F_{zz}^Q(\mathbf{p}',\omega)w(\mathbf{p}))\right]\right\} \tag{3}$$

Here $\mathbf{p}' = \mathbf{p} + \mathbf{g}$, $w(\mathbf{p}) = 2J\gamma(\mathbf{p}) = 2J\sum_i\cos(p_i)$ is the Fourier transform of the interaction, the summation is over the Matsubara frequencies $\omega_n = 2\pi n/\beta$, the $(d-1)$ dimensional integral is restricted to the surface Σ_Q defined by $\gamma(\mathbf{p}) = -\sqrt{d^2 - Q^2}$ and the functions $F_{ij}^Q(\mathbf{p},\omega) = <S^i(\mathbf{p},\omega)S^j(-\mathbf{p},-\omega)>$ are the Fourier transforms of the spin-spin dynamical correlation functions (in imaginary time) for a system where only fluctuations of wavevector $\mathbf{p}$ such that $|\gamma(\mathbf{p})| < \sqrt{d^2 - Q^2}$ are included. The isotropy of the model implies $F_{yy} = F_{xx}$ and $F_{yx} = -F_{xy}$. Analogous equations can be derived for the many spin correlation functions of the model. The (infinite) set of differential equations forms the QHRT hierarchy. When $Q = d$, fluctuations are neglected and the exact initial condition for the first QHRT equation (3) coincides with the mean field free energy density. The magnetic structure factors at $Q = d$ can be explicitly written as:

$$F_{xx}^Q(\mathbf{p},\omega) = \frac{\mu_\perp - w(\mathbf{p})}{m^{-2}\omega^2 + \mu_\perp^2 - w(\mathbf{p})^2};$$

$$F_{xy}^Q(\mathbf{p},\omega) = \frac{m^{-1}\omega}{m^{-2}\omega^2 + \mu_\perp^2 - w(\mathbf{p})^2};$$

$$F_{zz}^Q(\mathbf{p},\omega) = \frac{\delta_{\omega,0}}{\mu_{||} + w(\mathbf{p})} \tag{4}$$

where m is the staggered magnetization and $\mu_\perp$, $\mu_{||}$ are known functions of m. For $S = 1/2$: $\mu_\perp = 2T\, m^{-1} \tanh^{-1}(2m)$ and $\mu_{||} = 4T(1-4m^2)^{-1}$. Note that the dependence of the transverse magnetic structure factors in (4) on frequency and momentum is consistent with the first order spin wave result at zero temperature and reproduces the known single mode approximation which well represents antiferromagnetic correlations at low temperatures [9,10]. The longitudinal correlations in equation (4) are instead purely classical and, as such, satisfy the relationship $T\chi_{||}(k) = S_{||}(k)$ between longitudinal susceptibility $\chi_{||}(k)$ and the corresponding static structure factor $S_{||}(k)$.

Equation (3), although formally exact, is not closed because the evolution of the free energy depends on the unknown magnetic structure factors of the model $F_{ij}^Q(\mathbf{p}, \omega)$. Therefore, we have to introduce some approximate parametrization of the structure factors in terms of the free energy. The simple approximation we have studied is to retain the form of $F_{ij}^Q(\mathbf{p}, \omega)$ as given in Eq. (4) but imposing thermodynamic consistency in order to determine the two scalar parameters $\mu_\perp$ and $\mu_{||}$. More precisely, for every Q we related the transverse and longitudinal staggered susceptibilities to the free energy via the exact sum rules:

$$
\begin{aligned}
(\mu_\perp - 2dJ)^{-1} &= F_{xx}^Q(\mathbf{g}, \omega = 0) = m(\partial a^Q/\partial m)^{-1} \\
(\mu_{||} - 2dJ)^{-1} &= F_{zz}^Q(\mathbf{g}, \omega = 0) = (\partial^2 a^Q/\partial m^2)^{-1}
\end{aligned}
\tag{5}
$$

From the adopted structure of the dynamical correlation functions, we also obtain the relationship between the parameters entering F_{ij}^Q and the zero temperature non linear sigma model coupling constants: uniform transverse susceptibility $\chi_0 = 1/(4d)$, spin wave velocity $c = \sqrt{4d}\, m$ and spin stiffness $\rho_s = m^2$. The hydrodynamic relation $\chi_0 c^2 = \rho_s$ is automatically satisfied by our ansatz for arbitrary spontaneous magnetization m. It is interesting to note that from our parametrization, the scaling of the spin wave velocity c on approaching the critical temperature $(t = (T_c - T)/T_c \to 0)$ gives $c \propto m$ that is $c \propto t^\beta$ along the coexistence curve. The dynamic scaling hypothesis instead predicts $c \propto t^{\nu(z-1)}$ where z is the dynamical critical exponent. By use of scaling laws and recalling that in our approximation the correlation critical exponent vanishes ($\eta = 0$), we get $z = d/2$ which is the expected result for an antiferromagnet (i.e. model G) [11]. Equation (3), together with (4) and (5) give rise to a partial differential equation for the free energy density of the Heisenberg model $a^Q(m)$ as a function of the cut-off Q and of the magnetization m. The frequency sum can be carried out analytically giving the final equation:

$$
\frac{d\,a^Q}{dQ} = \frac{1}{2\beta} \int_{\mathbf{p} \in \Sigma_Q} \left\{ 4 \ln \left[\frac{\sinh\left(\frac{1}{2}\beta m \mu_\perp\right)}{\sinh\left(\frac{1}{2}\beta m \sqrt{\mu_\perp^2 - w(\mathbf{p})^2}\right)} \right] + \ln \left[\frac{\mu_{||}^2}{\mu_{||}^2 - w(\mathbf{p})^2} \right] \right\}
\tag{6}
$$

We numerically solved this partial differential equation for several values of the spin S and different temperatures in order to study the phase diagram of this system. Note that S just enters the theory through the initial condition $a^Q(m)$ at $Q = d$, while the form of the differential equation is unaffected by S. Before showing the numerical results, however, it is useful to discuss the behavior of Eq. (6) near a phase transition. In particular, we studied the neighborhood of the critical point (in $d > 2$) and the low temperature region. Both at the critical point and along the coexistence curve the susceptibilities diverge due to the presence of critical fluctuations and Goldstone bosons, respectively. From Eq. (5) we conclude that at long wavelengths (i.e. $Q \to 0$) and near a phase transition we have $\mu_\perp \sim \mu_{||} \sim 2dJ$. In this region equation (6) simplifies and, by rescaling the free energy as $a^Q Q^{-d}$ and the magnetization as $mQ^{(2-d)/2}$, it reduces to the RG equation obtained by Stanley $et\ al.$ [12] for a $O(3)$ symmetric ϕ^4 hamiltonian. Such an equation has been analyzed near four dimension and proved to give the correct critical exponents to first order in the $\epsilon = 4 - d$ expansion. In three dimensions, the numerical solution of the universal fixed point equation gives for the correlation length critical exponent the result $\nu = 0.826$, to be compared with the accepted value $\nu = 0.71$. The other critical exponents follow from the scaling laws, noting that our analytical form of the two point functions (4) forces the anomalous dimension exponent to vanish $\eta = 0$. We therefore find non classical exponents in three dimensions. Special care must be paid when dealing with the $T \to 0$ limit of our equation. In this case, the asymptotic form of the equation changes and it can be shown to give rise, near a hypothetical quantum critical point, to critical exponents appropriate for a $O(3)$ model in $d+1$ dimensions as expected. A separate analysis should be carried out in the low temperature phase. If symmetry is spontaneously broken, following Chakravarty $et\ al.$ [13], we may ask how quantum and thermal fluctuations modify the zero field magnetization. In order to answer this question we perform a Legendre transform on our equation (6): we first derive it with respect to the magnetization m obtaining an evolution equation for the magnetic field $h^Q(m)$ at fixed m. Then we find the equation governing the evolution of the spontaneous magnetization m^Q implicitly defined by the requirement $h^Q(m^Q) = 0$ at every Q. This procedure gives rise to a differential equation for m^Q. In the $Q \to 0$ limit, taking into account that the longitudinal susceptibility diverges more slowly than Q^{-2}, QHRT reduces to a simple ordinary differential equation:

$$\frac{dm^Q}{dQ} = K_d \left(\frac{Q}{\sqrt{d}} \right)^{d-2} \left[\tanh \left(Q\beta m^Q \right) \right]^{-1} \tag{7}$$

where K_d is a geometrical factor (ratio between the solid angle and volume of the Brillouin zone). By introducing the rescaled variable $g = \sqrt{4d}(Q/\sqrt{d})^{d-1}/m^Q$, equation (7) becomes identical, to order g^2, to the known weak coupling RG equations for the non linear sigma model applied by Chakravarty *et al.* [13] to the analysis of the antiferromagnetic Heisenberg model at long wavelengths and low temperatures. As an example, we plot in Fig. 1 the RG flux of g^Q obtained by the integration of the *full* QHRT equation (6). We clearly see the effect of the unstable zero temperature weak coupling fixed point while, for the nearest neighbor Heisenberg model, the other fixed point (g_c), governing the quantum critical regime, has no effect on the RG trajectories. This analysis shows that the single mode approximation to QHRT reproduces the correct long wavelength structure both near four and two dimensions. Furthermore, we expect QHRT to be superior to the weak coupling renormalization group equations because our non perturbative approach also describes the critical region and the high temperature regime where $m^Q \to 0$ as $Q \to 0$, corresponding to $g \to \infty$ i.e. to the strong coupling phase of the non linear sigma model.

Finally, we present few results of the numerical integration of Eq. (6) in three dimensions. As already pointed out in the classical case [6], the HRT approach is able to correctly implement Maxwell construction at first order phase transitions and in fact the free energy density $a^Q(m)$ at the end of the integration, i.e. in the $Q \to 0$ limit, becomes rigorously flat in a finite region of the magnetization axis for $T < T_c$. Therefore it is easy to extract from the numerical output the critical temperature and the coexistence curve, shown in Fig. 2 for several values of the spin S. The zero temperature limits of this curve agree within about 2% with the accepted estimates based on spin wave theory, Monte Carlo simulations or series expansions. Regrettably, for the spontaneous magnetization at finite temperature there are just few available results going beyond mean field approaches. Simulation data for the classical $S \to \infty$ case [14] and recent series expansion for the $S = 1/2$ model [15] seem to give somewhat larger coexistence regions. However, we believe that a more systematic analysis of these models by accurate numerical techniques is necessary before reaching a definite conclusion on the accuracy in the determination of the coexistence curve. The critical temperature for the classical model is known by several methods [5,16] to be $T_c = 1.443\,J$ while for the $S = 1/2$ case it has been recently estimated as $T_c = 0.946\,J$ [4] by use of a newly developed Quantum Monte Carlo method and $T_c = 0.93\,J$ [15] by series expansions. Our results are a few percent lower, being $T_c = 1.419\,J$ for $S = \infty$ and $T_c = 0.90\,J$ for $S = 1/2$. From the solution of the QHRT equation we also obtain other important information on the model, for instance, the equation of state, the specific heat and also the temperature dependent dynamical structure factors, via analytic continuation of the adopted expressions (4). In order to improve the QHRT results we have just discussed, other approximate expressions for the magnetic structure factors should be examined, possibly keeping the same form (4) but allowing for a non trivial renormalization factor for the uniform susceptibility. This method can be applied in a straightforward way to other models of interest in quantum many body physics, like the Hubbard model, and may help to determine the location of the magnetic phase transitions and the possible occurrence of phase separation in a purely repulsive electron system.

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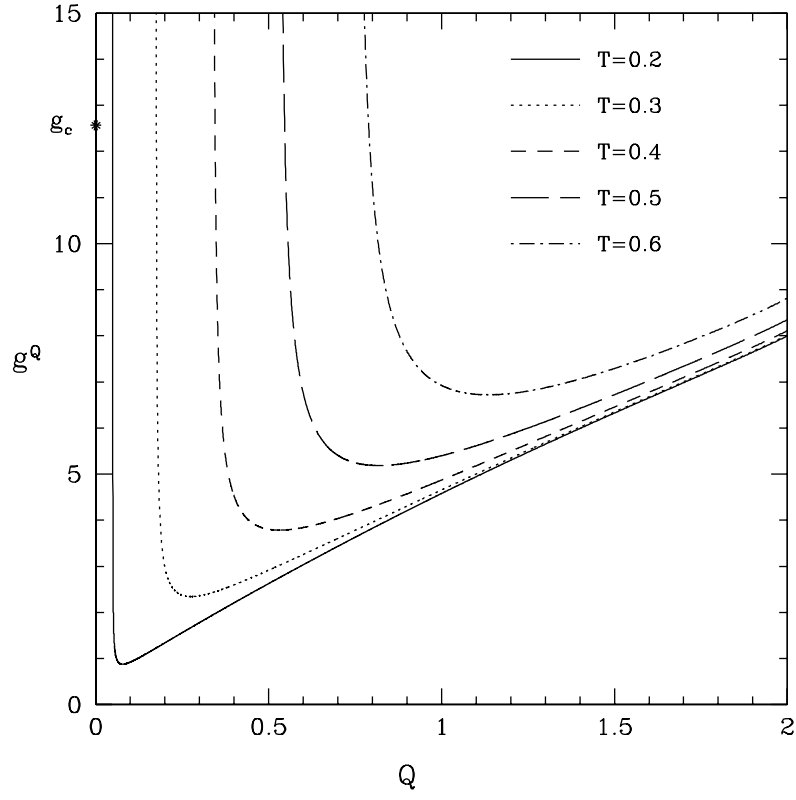
FIG. 1. RG trajectories for the two dimensional Heisenberg model computed via numerical integration of the QHRT equation.
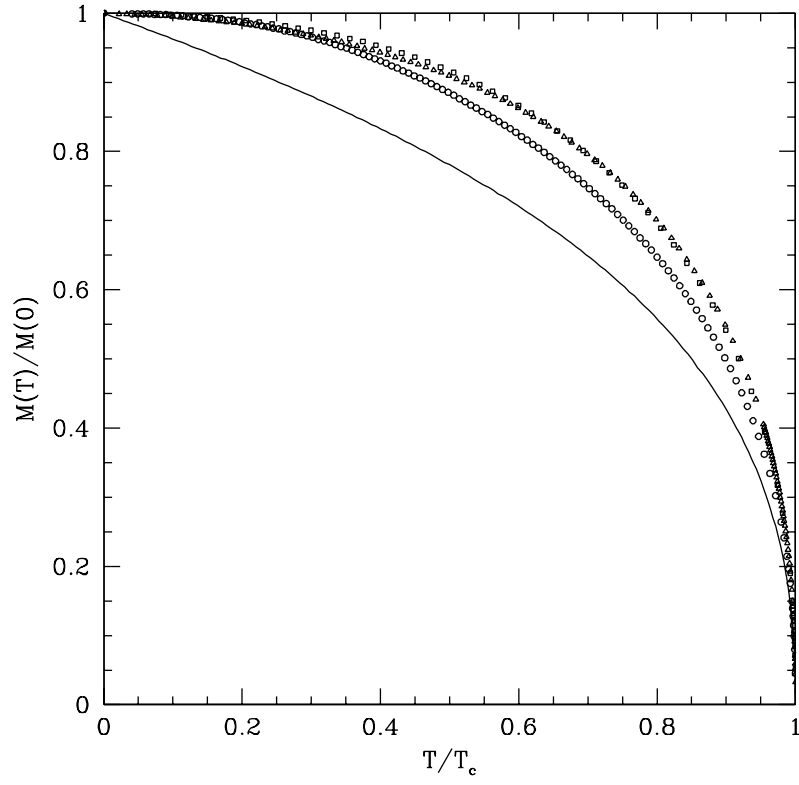
FIG. 2. Reduced spontaneous magnetization as a function of temperature for different values of the spin: $S = 1/2$ (triangles) $S = 1$ (squares) $S = 5/2$ (circles) and $S = \infty$ (full line).